Preprint
UCRL-JC-144174

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This article was submitted to
International Groundwater Symposium – Bridging the Gap between Measurement and Modeling in Heterogeneous Media
Berkeley, CA
March 25-28, 2002

U.S. Department of Energy

Lawrence
Livermore
National
Laboratory

August 8, 2001

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Implementation of Deterministically-Derived Hydrostratigraphic Units into a 3D Finite Element Model at the Lawrence Livermore National Laboratory Superfund Site

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ABSTRACT

Lawrence Livermore National Laboratory (LLNL) is a large Superfund site in California that is implementing an extensive ground water remediation program. The site is underlain by a thick sequence of heterogeneous alluvial sediments. Defining ground-water flow pathways in this complex geologic setting is difficult. To better evaluate these pathways, a deterministic approach was applied to define hydrostratigraphic units (HSUs) on the basis of identifiable hydraulic behavior and contaminant migration trends. The conceptual model based on this approach indicates that groundwater flow and contaminant transport occurs within packages of sediments bounded by thin, low-permeability confining layers. To aid in the development of the remediation program, a three-dimensional finite-element model was developed for two of the HSUs at LLNL. The primary objectives of this model are to test the conceptual model with a numerical model, and provide well field management support for the large ground-water remediation system. The model was successfully calibrated to 12 years of ground water flow and contaminant transport data. These results confirm that the thin, low-permeability confining layers within the heterogeneous alluvial sediments are the dominant hydraulic control to flow and transport. This calibrated model is currently being applied to better manage the large site-wide ground water extraction system by optimizing the location of new extraction wells, managing pumping rates for extraction wells, and providing performance estimates for long-term planning and budgeting.

INTRODUCTION

Lawrence Livermore National Laboratory (LLNL) is located in Livermore, California, about 50 miles east of San Francisco. The LLNL facility is a highly developed research and industrial facility that covers about 1 square mile. The site was converted from agricultural use into a Navy Air Field in 1942. In 1951, the site became a weapons design and basic physics research laboratory. In 1982, multiple plumes of volatile organic compounds (VOCs), predominantly trichloroethene (TCE) and tetrachloroethene (PCE), were discovered in ground water beneath LLNL. Prior to remediation, the plumes situated on the western margin of the site extended up to 4,000-ft offsite toward municipal supply wells in the city of Livermore.

In 1987, LLNL was placed on the U.S. Environmental Protection Agency's National Priority List. The environmental investigation covers an area of about 2 square miles to depths over 300 ft. As part of the environmental cleanup activities, LLNL operates a large ground water extraction system to remediate the VOC plumes beneath the site. In 2000, this system included a total of 80 ground water extraction wells connected to 25 separate treatment facilities. These combined facilities treated about 308 million gallons of ground water at an average combined flow rate of 600 gpm, and removed about 270 kg of VOCs in 2000. To better manage this large complex remediation system, a finite-element numerical model was developed.

CONCEPTUAL MODEL

Geologic Setting

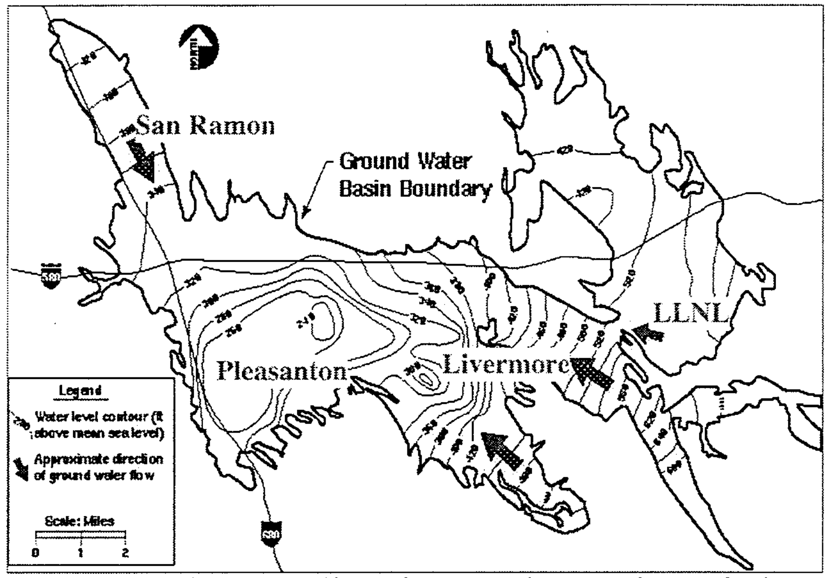

Figure 1: The Livermore Valley forms a major ground water basin

The Livermore Valley forms a ground water basin that is a significant water resource for the Livermore and Pleasanton areas (Figure 1). Within the basin, ground water flow is primarily from east to west. The primary areas of ground water discharge are along streams and pumping from wells. Water can only exit the valley as surface water through Niles Canyon in the southwestern corner of the valley. Average precipitation in the valley is about 14 inches per year (DWR 1966). The valley has historically been devoted to agriculture, but much of this area has experienced rapid urbanization from expansion from the greater San Francisco Bay Area in recent years.

LLNL is located in the eastern Livermore Valley (Figure 1). The Livermore Valley is a fault-bounded basin that is considered a Late Tertiary pull-apart basin that lies within the Coastal Range Province of California (DWR 1966). The sedimentary sequence within the primary alluvial aquifer consists of up to 1,000 ft of interbedded sands, gravels, silts, and clays within a sequence of Quaternary and Plio-Pleistocene alluvial fan, fluvial, and lacustrine deposits of the Livermore Formation (DWR 1966, Carpenter et al. 1984). The VOC plumes are contained within the upper 200 to 300 ft of sediments beneath LLNL. During initial studies at this site, the alluvial sequence was considered so heterogeneous that it could not be correlated or subdivided into ground water units, on a site-wide basis, that were relevant to the proposed ground water remediation (Thorpe et al. 1990).

Hydrostratigraphic Units

A hydrostratigraphic unit (HSU) is defined in this paper as a subsurface unit that is characterized by ground water flow that can be demonstrated to be distinct under both unstressed (natural) and stressed (pumping) conditions, and is distinguishable from flow in other HSUs (Noyes et al. 2000, in press). A deterministic approach was used to define HSUs at LLNL based on identifiable hydraulic behavior and contaminant migration trends using a systematic analysis of independent data sets. Using this approach, groundwater flow and contaminant transport were found to occur within packages of sediments bounded by thin, low-permeability confining layers. These layers were found to significantly limit hydraulic communication between the HSUs even after years of pumping. Based on extensive field data, these thin layers form the primary hydraulic controls within the alluvial sediments at LLNL (Noyes et al. 2000, in press).

For this deterministic approach to defining HSUs, a systematic, integrated analysis of the large, detailed data sets available at LLNL was performed. These data sets include an extensive history of long-term (constant flow tests over 8 hours) hydraulic testing that were particularly valuable in defining HSUs by categorizing the hydraulic responses of observation wells screened throughout the sequence. Other important data sets include monthly ground water elevations, ground water chemistry data, soil chemical data, and borehole lithologic and geophysical logs. The active LLNL ground water extraction systems also now serve as another data set that monitors the hydraulic responses in wells over a period of years. As a result of this analysis, 9 HSUs have been defined at LLNL (Figure 2). The primary assumption of the conceptual model is that between these confining layers, if fully saturated, the ground water is considered to be relatively well mixed and that ground water flow and contaminant transport is essentially parallel to the HSU boundaries (Noyes et al. 2000, in press).

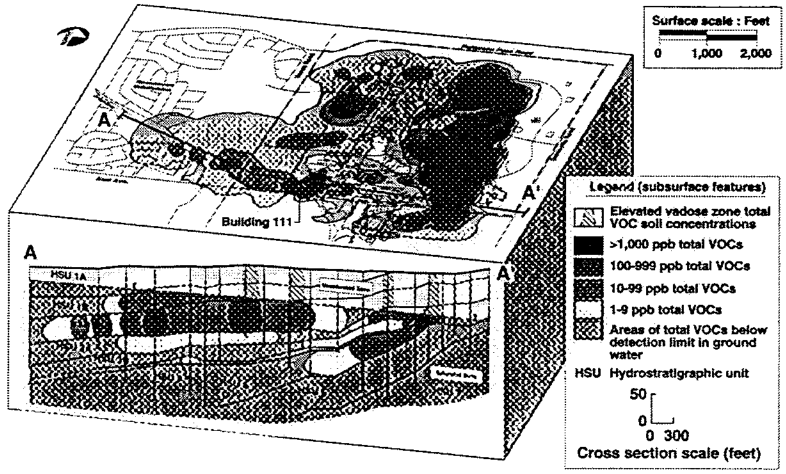

Figure 2: Hydrostratigraphic conceptual model for LLNL.

NUMERICAL MODEL

Approach

To enhance subsurface remediation efforts, a finite-element flow and transport model using FEFLOW (Diersch, 1998) was developed for HSUs 1B and 2. HSUs 1B and 2 are the most impacted by VOC plumes on the western side of LLNL, and extend offsite, so they are of particular interest to the LLNL cleanup activities. These HSUs also have a relatively consistent geologic character across the site making them more suitable for regional scale modeling. The confining layer was simulated as a thin low-permeability layer. By including the HSU boundary, the model is also designed to verify whether a numerical model can simulate the current conceptual model of thin confining layers separating the HSUs by matching the observed field data. The model was calibrated over 10 years of historical flow and VOC plume data.

Model Setup

The numerical model domain is set in the Eastern Livermore Valley and covers an area of about 7 square miles (Figure 1). The model is constructed of 13 elemental layers and 14 nodal slices (Figure 3). Elemental layers 1 through 6 represent HSU 1B; layer 7 is the thin confining layer; and layers 8 through 13 represent HSU 2. The increased vertical resolution allows for better resolution of partial saturation areas, and provides

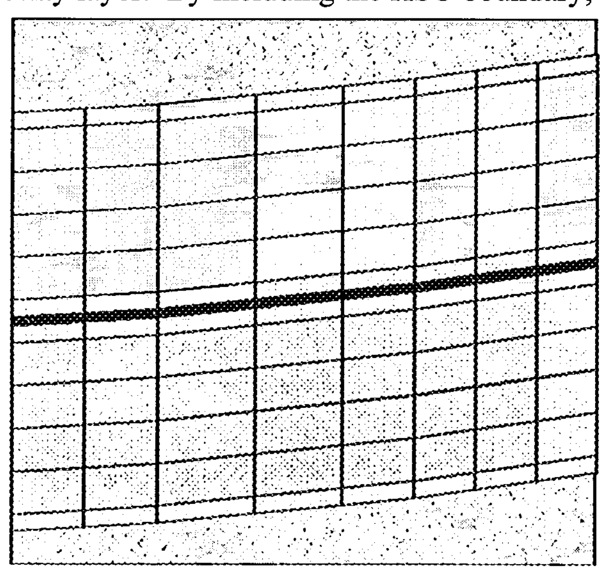

Figure 3: Vertical profile of numerical FEFLOW model

higher resolution in areas with significant hydraulic and chemical gradients between HSUs. The HSU thickness was based on sitewide correlations and was subdivided equally across the elemental layers. HSU 1B is typically about 50 ft thick, and HSU 2 is typically about 70 ft thick. The thin confining layer was uniformly set to 1 ft thick. The model domain was discretized into 31,636 tri-lateral finite elements per layer and 15,922 nodes per layer for a total of 222,908 nodes within the entire model. Horizontal nodal spacing varied from 15 ft in areas with high VOC concentration areas to a maximum of 375 ft in non-contaminated areas. Mesh refinement was done to improve model accuracy and to minimize potential numerical errors.

The model was simulated with steady-state flow and transient transport under confined conditions. To account for temporal variation of boundary conditions, the model was separated into 36 stress periods for the calibration period of April 1988 to December 2000. Early stress periods from 1988 through 1995 varied from 4 to 12 months, whereas after 1995, stress periods were uniformly 3 months. These stress periods are primarily related to changes in the extensive LLNL ground water extraction system.

Boundary Conditions and Aquifer Parameters

The deterministic approach was also applied in the development of boundary conditions and aquifer parameters. The major hydrogeologic features within the model domain are shown on Figure 4. Boundary conditions for these features were defined based on available historical data. In the northwestern section of the domain, ground water directly discharges into Arroyo Las Positas. Stream gage data indicates that Arroyo Las Positas has about 1,000 ft of gaining reach in this area with a discharge of about 0.8 cubic ft per second. Because of potential measurement error, the discharge rate was considered a general target and was considered a calibration parameter. After calibration, the discharge was distributed 75% to HSU 1B and 25% to HSU 2.

Along the eastern edge of the domain, a constant-head boundary condition was applied to represent influx from a drainage system in the hills to the east. The constant head value was applied to HSU 2 only, and was based on hydrographs from nearby observation wells. Along the southwestern edge of the domain, the interconnection with the adjacent part of the ground water basin is impacted by a thin fault block. A narrow opening in this block connects these two basins and is referred to as the Gap. A constant head boundary condition was applied to both HSUs 1B and 2, and was based on hydrographs from nearby observation wells. The northern boundary is considered a no-flow boundary that represents a ground water divide. The other boundaries are considered no-flow boundaries that represent the fault-bounded edge of the ground water basin.

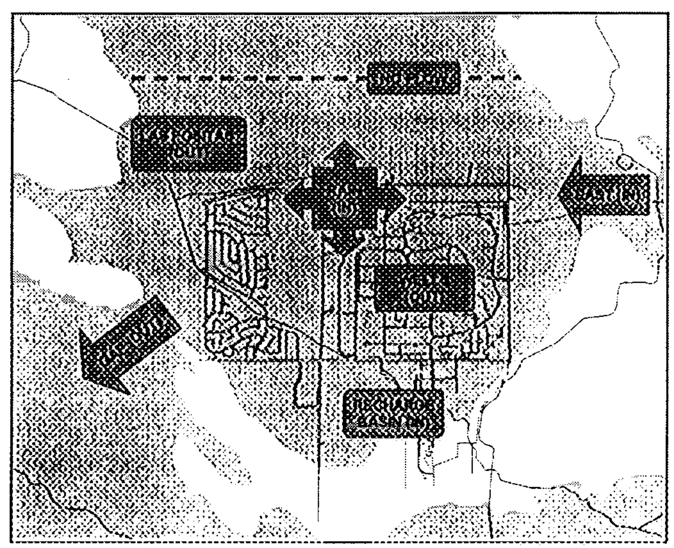
Figure 4: Ground water model domain with major boundary conditions

Recharge from rainfall was generally applied to HSU 1B. However, in the eastern section of the domain, HSU 2 is the first saturated HSU. In these areas, recharge was allowed to directly impact HSU 2. A database of monthly ground water extraction volumes for the 80 LLNL extraction wells and 2 known agricultural wells was constructed for the entire calibration history, and was directly input into the numerical model. A portion of the extracted ground water from LLNL is put back into the aquifer using a recharge basin located to the south of LLNL. Monthly data exists on the volume pumped to the recharge basin, and that water was distributed equally between HSU 1B and 2 in the model.

Hydraulic conductivity was based on observed permeability trends and hydraulic test data. Hydraulic conductivity was the primary calibration parameter and the calibrated values range from 0.0035 to 0.0045 cm/s in HSU 1B and 0.0005 to 0.0045 cm/s in HSU 2. Hydraulic conductivity generally increases from east to west. The thin confining layer had a uniform hydraulic conductivity of 0.0000001 cm/s. Retardation coefficients were obtained from Bishop et al. (1989). Diffusion and decay were considered negligible. The model did not incorporate any contaminant source terms.

MODEL RESULTS

Flow Calibration

Primary emphasis was placed on calibrating the ground water flow model with the assumption that ground water velocities were the primary mechanism that controlled contaminant transport at LLNL. The flow model was calibrated in two steps. The first calibration step was performed with 8 stress periods, and the calibration focused primarily on obtaining a hydraulic conductivity distribution. These 8 stress periods were selected to represent distinct boundary conditions and ground water extraction rates. The goal was to define a single hydraulic conductivity distribution for each HSU that would apply under all conditions experienced at the site through time. The initial hydraulic conductivity estimations were determined by a non-linear parameter estimation (PEST) method (Dougherty, 1994) that is included as a module within FEFLOW. By using visual and analytical methods, a set of unique hydraulic conductivity zones was established for the entire simulation period by calibrating to measured ground water elevations for that stress period. Once hydraulic conductivity estimates were established, boundary conditions and other aquifer parameters were adjusted using PEST or trial and error methods to improve differences between observed and modeled peizometric surfaces for these 8 stress periods.

The second calibration step was to extend the ground water elevation matching to all 36 steps. A major task for this step was the development of consistent set of ground water elevation maps for each HSU. The primary calibration parameters were hydraulic conductivity, surface recharge,

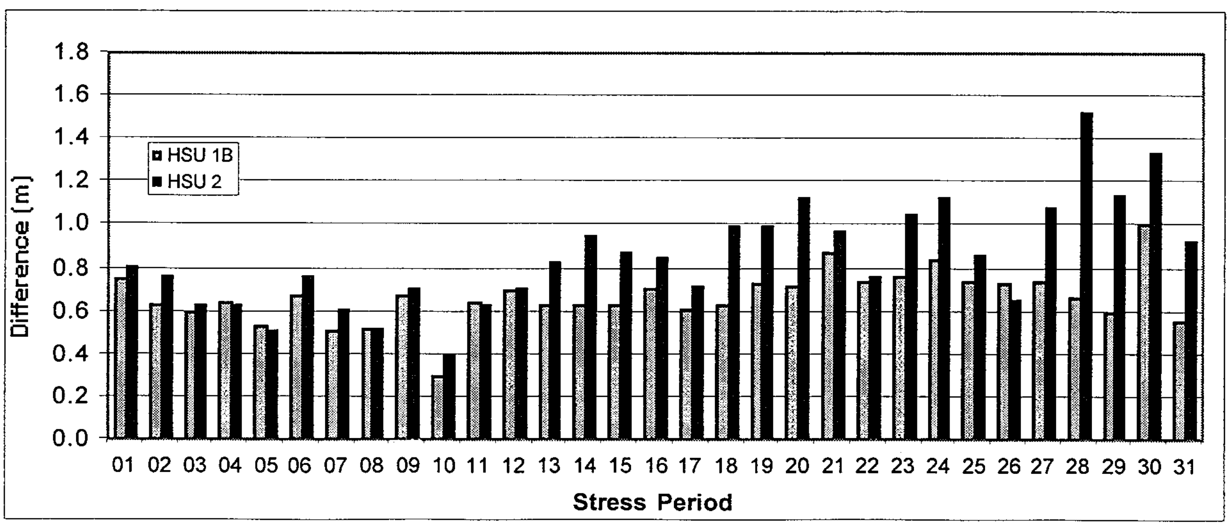

Figure 5: Absolute integrated difference (L1) for HSU 1B and 2 for calibrated FELOW model

and discharge to Arroyo Las Positas. The constant head boundary conditions and wells were based on measured data and considered to be fixed values. There is overall good agreement between measured and predicted results over the entire model domain for all stress periods (Figure 5). These variations mostly represent shifts in ground water elevation, but the overall hydraulic gradient was preserved. The cause of these shifts is due in part to 1) differences between the model based on average conditions over a stress period whereas the ground water elevations represent a distinct time within the stress period, 2) the model assumes steady-state conditions whereas the measured data may represent a transient condition, and 3) the model boundary conditions and aquifer parameters have been smoothed and regionalized to some degree whereas the measured data may represent more local heterogeneity. Improvements in the flow calibration would be anticipated if these issues are addressed.

Transport Calibration

Groundwater velocities from the flow model were used as input for the contaminant transport model. To calibrate the transport model, initial TCE and PCE source plumes were modeled forward and compared to quarterly plume maps from December 1991 to December 2000. A major task for this step was the development of consistent set of TCE and PCE plume maps for each HSU. For this task, a decision-based algorithm was developed that integrates multiple chemistry data sets over time to establish a consistent set of plume maps over the entire calibration interval. These maps were verified with site hydrogeological interpretations to maintain accuracy and consistency. The transport model was calibrated by visual comparison of model simulations and these quarterly maps. Where discrepancies were noted, adjustments were made in either the flow model or in transport parameters. This process was repeated until an overall good agreement between observed and predicted plumes of PCE and TCE was achieved. By history matching TCE and PCE data from 10 years of remediation, the model was considered capable of making accurate forecasts of conditions into the future. Therefore the numerical model was able to provide decision support for wellfield management and other remediation decisions. In addition, the history matching by the transport model provided additional confirmation that the thin confining layer from the conceptual model represents field conditions.

Application

The calibrated FEFLOW flow and transport model is currently being applied at LLNL to optimize ground water remediation efforts and to support long-range planning and budgeting for the Superfund cleanup activities. For example, budget managers had proposed that LLNL shift from an more aggressive cleanup to a "cheap-to-keep" strategy. The proposal was that annual operating costs would be reduced by operating a small number of wells along the site boundary. The model was able to provide input to evaluate the long-range costs by demonstrating that the aggressive strategy would require 50 years to get all but the source areas below regulatory levels whereas the "cheap-to-keep" strategy would require over 250 years.

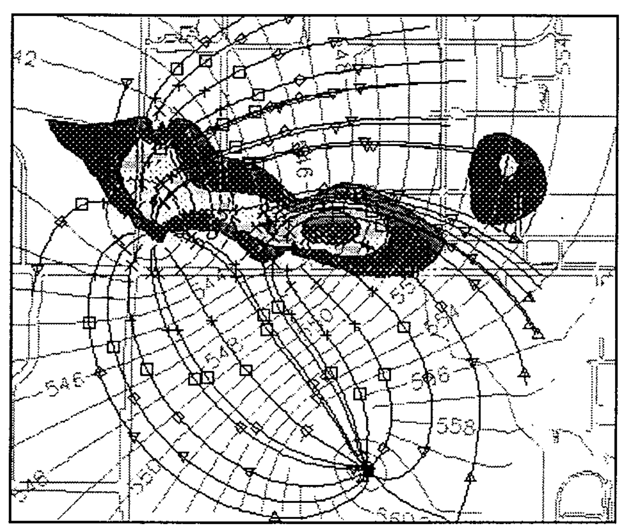

Figure 6: Capture zone analysis for HSU 1B, Treatment Facility A

As a second example, the model has been useful in evaluating the complex extraction well interference patterns in the southwestern portion of LLNL (Figure 6). This is the area where an offsite plume once extended over 4000 ft offsite. In this area, 7 wells in HSU 1B and 13 wells in HSU 2 pump at a cumulative pumping rate of over 350 gpm. The extracted ground water from this area is returned to the ground water basin through a recharge basin located 1,500 ft to the south. The model has proven useful for wellfield management to adjust flow rates in wells to keep stagnation points from inhibiting cleanup of this area. Current modeling scenarios include capture zone analysis, pumping interference evaluation, extraction well placement, optimal pumping rates, mass removal projections, and long-range remediation assessment. In one case, the model was used to choose a well in which to install a larger pump, thereby avoiding the additional cost of re-installing the pump using a trial and error approach.

DISCUSSION

The identification of thin confining layers within heterogeneous alluvial sediments is not widely recognized. Initial geologic descriptions of these layers did not note anything remarkable. However, once the hydrostratigraphic relationships were determined, it became clear that the plumes were residing within distinct flow systems. Current research indicates that the HSU boundaries at LLNL correspond to paleosol layers; however, numerous paleosols were found within the vertical sequence beneath LLNL (Weissman et al. 2000). It is currently postulated that certain of these paleosol layers are laterally continuous enough to form competent confining layers across the site. Research is continuing in defining the nature of the HSU boundaries at LLNL (Weissman et al. 2000, Karachewski et al. 2000). This concept of thin confining layers forming significant hydraulic controls within alluvial sediments may apply to locations other than the Eastern Livermore Valley. A similar setting was noted in the Kings River Fan of Central California (Weissman and Fogg 1999; Weissman et al. in press).

Using a deterministic approach was successful in developing the conceptual and numerical models in a time frame where the model could be employed to provide a useful evaluation tool for engineering decisions for this project. The deterministic approach to defining HSUs and model setup is based on careful analysis and integration of the available data sets. At LLNL, the extensive environmental restoration project has generated a large, complete data set. Importantly, the data set contains a large amount of hydraulic test data, monthly water levels, ground water chemistry, and extraction well histories. We have found that this data has been important to understanding the conceptual model and building the numerical model. Work is continuing on developing the conceptual and numerical models at LLNL. Future work includes defining the heterogeneity within an HSU and how to represent that in a numerical model, developing numerical models for the more geologically complex deeper HSUs, and incorporating more detailed hydrogeological data sets into the model.

CONCLUSIONS

The deterministic approach taken was successfully applied to handle a large and complex data set and develop a model for a large remediation site. This deterministic approach was used for the development of both the conceptual and numerical models. Through detailed analysis, a conceptual model was defined based on field observation that flow and transport is contained between thin confining layers within the heterogeneous alluvial sediments, and little communication occurs across them. The numerical model was successfully calibrated to measured ground water elevation and plume maps. Through this calibration, the impact of this thin confining layer was simulated which provided additional confirmation that this conceptual model is appropriate for LLNL. The calibrated model has been applied to support wellfield management decisions and provide future performance evaluations for long-range planning and budgeting.

ACKNOWLEDGEMENTS

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48. The authors also would like to thank Charles Noyes of LLNL for support with the conceptual model, Jacob Bear of Technion Institute for ongoing support of modeling projects at LLNL, Souheil Ezzedine of Weiss Associates for support on numerical solutions, and Gary Weissman of Michigan State University for work on the nature of HSU boundaries.

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